Rapid Communications

Conserved spin current for the Mott relation

Cong Xiao, Jihang Zhu, Bangguo Xiong, and Qian Niu

Department of Physics, The University of Texas at Austin, Austin, Texas 78712, USA

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The conserved bulk spin current [Shi *et al.*, Phys. Rev. Lett. **96**, 076604 (2006)], defined as the time derivative of the spin displacement operator, ensures automatically the Onsager relation between the spin Hall effect (SHE) and the inverse SHE. Here, we reveal another desirable property of this conserved spin current: the Mott relation linking the SHE and its thermal counterpart, the spin Nernst effect (SNE). According to the Mott relation, the SNE is known once the SHE is understood. In a two-dimensional Dirac-Rashba system with a smooth scalar disorder potential, we find a sign change of the spin Nernst conductivity when tuning the chemical potential.

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In the rapidly expanding fields of spintronics and spin caloritronics, the spin Hall effect (SHE) [1,2] and its thermal counterpart, the spin Nernst effect (SNE) [3–11], have played important roles. When describing the SHE and SNE in terms of the bulk spin current in the presence of a band-structure spin-orbit interaction, there exists a well-known ambiguity about the definition of a transport spin current when the transported spin component is not conserved. A conserved bulk spin current has been proposed by Shi, Zhang, Xiao, and Niu (hereafter referred to as the SZXN spin current) [12,13] and has been studied intensively [14–21]. The SZXN spin current operator is described as the time derivative of the spin displacement operator (see below). The so-defined spin current has a natural conjugate force and represents a transport current. The Onsager relation can thus be established automatically between the SHE and inverse SHE of this SZXN spin current [12,14,18]. In this Rapid Communication, we reveal another desirable property of the SZXN spin current: the Mott relation between the SHE and SNE. The Mott relation [22] can be viewed as a fundamental link between the transport current responses to the electric field and to the temperature gradient in independent-carrier systems with elastic scattering off disorder. According to the Mott relation, the SNE is known once the SHE is understood.

As applications, we show that, in the weak disorder-potential regime, both the SHE and SNE can be finite in a two-dimensional (2D) Dirac-Rashba system with a smooth disorder potential, contrary to the vanishing SHE [20,21] and SNE in a Rashba 2D electron gas. A sign change of the spin Nernst conductivity is found when tuning the chemical potential.

Generalized Mott relation. The out-of-equilibrium average value of an observable $\hat{O}$ in a single-particle system reads $\delta O = \mathrm{Tr}\langle \hat{O}^{\mathrm{eq}}(\delta\hat{\rho})\rangle + \mathrm{Tr}\langle \hat{\rho}^{\mathrm{eq}}\delta\hat{O}\rangle$ in the linear response regime. Here, $\hat{\rho}$ is the single-particle density matrix with $\hat{\rho}^{\mathrm{eq}}$ and $\delta\hat{\rho}$ the equilibrium and linear-response components, respectively. $\hat{O}^{\mathrm{eq}}$ and $\delta\hat{O}$ have analogous meanings, and $\langle\cdots\rangle$ denotes the disorder averaging. The usual external perturbations driving nonequilibrium steady states in experiments are the electric field $\mathbf{E}$ and temperature gradient $-\nabla T/T$. For transport effects, the temperature gradient can be equivalently replaced by the gradient $-\nabla\psi/c^2$ of a fictitious gravitational potential ψ introduced by Luttinger (c is the speed of light) [23]. The first term of δO arises from the density-matrix linear response $\delta\hat{\rho} = \delta^{\mathbf{E}}\hat{\rho} + \delta^{\psi}\hat{\rho}$, whereas the second term comes from the linear response of the observable operator itself with respect to external perturbations $\delta\hat{O} = \delta^{\mathbf{E}}\hat{O} + \delta^{\psi}\hat{O}$. As a result, the linear response of any transport current $\hat{O}$ of a single-electron system with respect to the dc uniform $\mathbf{E}$ and $-\nabla\psi/c^2$ reads ($\alpha,\beta = x,y$)

$$\delta O_\alpha = L^{oe}_{\alpha\beta}E_\beta + L^{oQ}_{\alpha\beta}\left(\frac{-\partial_\beta\psi}{c^2}\right), \tag{1}$$

where $L^{o\xi}_{\alpha\beta} = D^{o\xi}_{\alpha\beta} + M^{o\xi}_{\alpha\beta}$ with $D^{oe}_{\alpha\beta}E_\beta \equiv \mathrm{Tr}\langle \hat{O}^{\mathrm{eq}}_\alpha \delta^{\mathbf{E}}\hat{\rho}\rangle$, $D^{oQ}_{\alpha\beta}(\frac{-\partial_\beta\psi}{c^2}) \equiv \mathrm{Tr}\langle \hat{O}^{\mathrm{eq}}_\alpha \delta^{\psi}\hat{\rho}\rangle$, $M^{oe}_{\alpha\beta}E_\beta \equiv \mathrm{Tr}\langle \hat{\rho}^{\mathrm{eq}}\delta^{\mathbf{E}}\hat{O}_\alpha\rangle$, and $M^{oQ}_{\alpha\beta}(\frac{-\partial_\beta\psi}{c^2}) \equiv \mathrm{Tr}\langle \hat{\rho}^{\mathrm{eq}}\delta^{\psi}\hat{O}_\alpha\rangle$. The basic considerations for obtaining $\delta^{\mathbf{E},\psi}\hat{\rho}$ and $\delta^{\mathbf{E},\psi}\hat{O}$ can be found in the classical treatment in Ref. [22], where the electric field enters the total single-carrier Hamiltonian $\hat{H}^t$ via the dipole term $-e\hat{\mathbf{r}}\cdot\mathbf{E}$. This is the case in the level of the full Hamiltonian [24,25], while in the level of an effective Hamiltonian, the canonical position $\hat{\mathbf{r}}$ may not be the physical one $\hat{\mathbf{r}}^{\mathrm{phy}}$ and an anomalous dipole $e(\hat{\mathbf{r}}^{\mathrm{phy}} - \hat{\mathbf{r}})$ (usually related to effective spin-orbit interactions [26,27]) couples to the electric field [24]. This situation needs a separate treatment [25,26]. In the present study we neglect this complexity and take $\hat{\mathbf{r}}^{\mathrm{phy}} = \hat{\mathbf{r}}$ approximately even when the transport is calculated in the level of effective Hamiltonians [28]. Thus the spin-orbit interactions with an external electric field and with a disorder potential [24–26] do not appear throughout this Rapid Communication.

$D^{o\xi}_{\alpha\beta}$ is generally given by the Bastin version of the $\hat{O}_\alpha - \hat{j}^{\xi}_\beta$ correlation function [29], which can be cast into [30]

$$D^{o\xi}_{\alpha\beta} = D^{o\xi,I(a)}_{\alpha\beta} + D^{o\xi,I(b)}_{\alpha\beta} + D^{o\xi,II}_{\alpha\beta} \tag{2}$$

with

$$D^{o\xi,I(a)}_{\alpha\beta} = -\frac{\hbar}{2\pi}\int d\epsilon \frac{df^0(\epsilon)}{d\epsilon}\mathrm{Tr}\big\langle \hat{O}^{\mathrm{eq}}_\alpha \hat{G}^R(\epsilon)\hat{j}^{\mathrm{eq},\xi}_\beta \hat{G}^A(\epsilon)\big\rangle,$$

$$D^{o\xi,I(b)}_{\alpha\beta} = \frac{\hbar}{2\pi}\mathrm{Re}\int d\epsilon \frac{df^0(\epsilon)}{d\epsilon}\mathrm{Tr}\big\langle \hat{O}^{\mathrm{eq}}_\alpha \hat{G}^R(\epsilon)\hat{j}^{\mathrm{eq},\xi}_\beta \hat{G}^R(\epsilon)\big\rangle,$$

and

$$D_{\alpha\beta}^{o\xi,II}=\frac{\hbar}{2\pi}\,\mathrm{Re}\int d\epsilon f^{0}(\epsilon)\mathrm{Tr}\left\langle \hat{O}_{\alpha}^{\mathrm{eq}}\hat{G}^{R}(\epsilon)\hat{j}_{\beta}^{\mathrm{eq},\xi}\frac{d\hat{G}^{R}(\epsilon)}{d\epsilon}-\hat{O}_{\alpha}^{\mathrm{eq}}\frac{d\hat{G}^{R}(\epsilon)}{d\epsilon}\hat{j}_{\beta}^{\mathrm{eq},\xi}\hat{G}^{R}(\epsilon)\right\rangle.$$

Here, $\hat{j}_{\beta}^{\mathrm{eq},\xi}$ stands for the equilibrium electric current ($\xi=e$) and heat current ($\xi=Q$) operators $\hat{j}_{\beta}^{\mathrm{eq},e}=e\hat{v}_{\beta}$, $\hat{j}_{\beta}^{\mathrm{eq},Q}=\frac{1}{2}\{\hat{H}^{\mathrm{eq}}-\mu,\hat{v}_{\beta}\}$. $\hat{G}^{R/A}(\epsilon)=(\epsilon-\hat{H}^{\mathrm{eq}}\pm i0^{+})^{-1}$ with $\hat{H}^{\mathrm{eq}}$ the single-particle Hamiltonian at equilibrium, f^{0} is the equilibrium Fermi distribution, and μ is the chemical potential. Now we derive a general relation between $D_{\alpha\beta}^{oQ}$ and $D_{\alpha\beta}^{oe}$. By using $(\hat{G}^{R/A})^{2}=-d\hat{G}^{R/A}/d\epsilon$, we get

$$D_{\alpha\beta}^{oQ,I(a)}=\int d\epsilon\left[-\frac{df^{0}(\epsilon)}{d\epsilon}\right]\frac{(\epsilon-\mu)}{e}D_{\alpha\beta}^{oe,I(a)}(T=0,\epsilon)+\frac{\hbar}{4\pi}\int d\epsilon\frac{df^{0}(\epsilon)}{d\epsilon}\mathrm{Tr}\langle\hat{O}_{\alpha}^{\mathrm{eq}}\hat{v}_{\beta}^{\mathrm{eq}}\hat{G}^{A}(\epsilon)+\hat{v}_{\beta}^{\mathrm{eq}}\hat{O}_{\alpha}^{\mathrm{eq}}\hat{G}^{R}(\epsilon)\rangle,$$

$$D_{\alpha\beta}^{oQ,I(b)}=\int d\epsilon\left[-\frac{df^{0}(\epsilon)}{d\epsilon}\right]\frac{(\epsilon-\mu)}{e}D_{\alpha\beta}^{oe,I(b)}(T=0,\epsilon)-\frac{\hbar}{4\pi}\int d\epsilon\frac{df^{0}(\epsilon)}{d\epsilon}\mathrm{Tr}\left\langle\frac{1}{2}\{\hat{O}_{\alpha}^{\mathrm{eq}},\hat{v}_{\beta}^{\mathrm{eq}}\}[\hat{G}^{R}(\epsilon)+\hat{G}^{A}(\epsilon)]\right\rangle,$$

and

$$D_{\alpha\beta}^{oQ,II}=-\int d\epsilon\left[f^{0}(\epsilon)+(\epsilon-\mu)\frac{df^{0}(\epsilon)}{d\epsilon}\right]\frac{1}{e}D_{\alpha\beta}^{oe,II}(T=0,\epsilon)+\frac{\hbar}{4\pi}\int d\epsilon\frac{df^{0}(\epsilon)}{d\epsilon}\mathrm{Tr}\left\langle\frac{1}{2}[\hat{O}_{\alpha}^{\mathrm{eq}},\hat{v}_{\beta}^{\mathrm{eq}}][\hat{G}^{R}(\epsilon)-\hat{G}^{A}(\epsilon)]\right\rangle,$$

then $D_{\alpha\beta}^{oQ}(T,\mu)=D_{\alpha\beta}^{oQ,I}(T,\mu)+D_{\alpha\beta}^{oQ,II}(T,\mu)$ yields the first main result of this Rapid Communication,

$$D_{\alpha\beta}^{oQ}(T,\mu)=\int d\epsilon\left[-\frac{df^{0}(\epsilon)}{d\epsilon}\right]\frac{(\epsilon-\mu)}{e}D_{\alpha\beta}^{oe}(T=0,\epsilon)-\frac{1}{e}\int d\epsilon f^{0}(\epsilon)D_{\alpha\beta}^{oe,II}(T=0,\epsilon). \tag{3}$$

On the other hand, utilizing $(\hat{G}^{R/A})^{2}=-d\hat{G}^{R/A}/d\epsilon$ and [30] $i\hbar\hat{G}^{R}\hat{v}_{\beta}^{\mathrm{eq}}=\hat{G}^{R}[\hat{r}_{\beta},\hat{H}^{\mathrm{eq}}]=\hat{G}^{R}[(\hat{G}^{R})^{-1},\hat{r}_{\beta}]$, we get

$$D_{\alpha\beta}^{oe,II}=\frac{e}{2}\int d\epsilon\frac{df^{0}(\epsilon)}{d\epsilon}\mathrm{Tr}\langle\{\hat{O}_{\alpha}^{\mathrm{eq}},\hat{r}_{\beta}\}\delta(\epsilon-\hat{H}^{\mathrm{eq}})\rangle+\frac{e}{\pi}\,\mathrm{Im}\int d\epsilon f^{0}(\epsilon)\mathrm{Tr}\langle\hat{O}_{\alpha}^{\mathrm{eq}}\hat{G}^{R}(\epsilon)\hat{r}_{\beta}\hat{G}^{R}(\epsilon)\rangle.$$

We find that, if the current $\hat{O}_{\alpha}$ is defined in terms of the time derivative of some displacement operators [12], i.e.,

$$\hat{O}_{\alpha}=\frac{1}{i\hbar}[\hat{F}_{\alpha},\hat{H}^{t}]\quad\text{where }[\hat{F}_{\alpha},\hat{r}_{\beta}]=0, \tag{4}$$

then $\mathrm{Tr}\langle\hat{O}_{\alpha}^{\mathrm{eq}}\hat{G}^{R}\hat{r}_{\beta}\hat{G}^{R}\rangle=\frac{1}{i\hbar}\mathrm{Tr}\langle[\hat{r}_{\beta},\hat{F}_{\alpha}]\hat{G}^{R}\rangle=0$ and

$$D_{\alpha\beta}^{oe,II}=\frac{e}{2}\int d\epsilon\frac{df^{0}(\epsilon)}{d\epsilon}\mathrm{Tr}\langle\{\hat{O}_{\alpha}^{\mathrm{eq}},\hat{r}_{\beta}\}\delta(\epsilon-\hat{H}^{\mathrm{eq}})\rangle. \tag{5}$$

For the current $\hat{O}_{\alpha}$ in the form of Eq. (4), one has $\delta^{\mathbf{E}}\hat{O}=0$ and $\delta^{\psi}\hat{O}=\frac{1}{2}\{\hat{r}_{\beta},\hat{O}^{\mathrm{eq}}\}\frac{\partial_{\beta}\psi}{c^{2}}$, thus $\delta O_{\alpha}=D_{\alpha\beta}^{oe}E_{\beta}+(D_{\alpha\beta}^{oQ}+M_{\alpha\beta}^{oQ})(\frac{-\partial_{\beta}\psi}{c^{2}})$, where $M_{\alpha\beta}^{oQ}(\frac{-\partial_{\beta}\psi}{c^{2}})\equiv\mathrm{Tr}\langle\hat{\rho}^{\mathrm{eq}}\delta^{\psi}\hat{O}_{\alpha}\rangle$ is given by [22]

$$\begin{aligned}M_{\alpha\beta}^{oQ}&=-\frac{1}{2}\int d\epsilon f^{0}(\epsilon)\mathrm{Tr}\langle\delta(\epsilon-\hat{H}^{\mathrm{eq}})\{\hat{r}_{\beta},\hat{O}_{\alpha}^{\mathrm{eq}}\}\rangle\\&=\frac{1}{e}\int d\epsilon f^{0}(\epsilon)D_{\alpha\beta}^{oe,II}(T=0,\epsilon).\end{aligned} \tag{6}$$

Combining Eqs. (5), (6), and (3) yields the generalized Mott relation

$$L_{\alpha\beta}^{oQ}(T,\mu)=\int d\epsilon\left[-\frac{df^{0}(\epsilon)}{d\epsilon}\right]\frac{(\epsilon-\mu)}{e}L_{\alpha\beta}^{oe}(T=0,\epsilon) \tag{7}$$

for the current $\hat{O}_{\alpha}$ having the form of Eq. (4). This relation is exactly the same as the well-known generalized Mott relation [22] between $L_{\alpha\beta}^{eQ}$ and $L_{\alpha\beta}^{ee}$. Equations (3)–(7) are the main result of this Rapid Communication. When the distances between the chemical potential and the band edges are much larger than the thermal energy $k_{B}T$, the Sommerfeld expansion is legitimate [31], yielding the standard Mott relation

$$L_{\alpha\beta}^{oQ}(T,\mu)/T=\frac{\pi^{2}k_{B}^{2}T}{3e}\frac{\partial L_{\alpha\beta}^{oe}(T=0,\epsilon)}{\partial\epsilon}\bigg|_{\epsilon=\mu}, \tag{8}$$

which relates $L_{\alpha\beta}^{oQ}$ to the energy derivative of $L_{\alpha\beta}^{oe}$ around the chemical potential.

Both the electric current operator $\hat{j}^{e}=e\frac{1}{i\hbar}[\hat{\mathbf{r}},\hat{H}^{t}]$ and the SZXN spin current operator $\hat{j}^{s}=\frac{1}{i\hbar}[\hat{\mathbf{r}}\hat{s}_{z},\hat{H}^{t}]$ have the form of Eq. (4). Thus the SNE of the SZXN current can be obtained once its SHE is known.

Applications. The intrinsic spin Hall conductivity $\sigma_{yx}^{s,\mathrm{in}}$ of the SZXN current can be obtained by the standard Kubo formula [12,14,17]. Aside from the intrinsic contribution, there exists a disorder-induced contribution to the SHE [1,2,20,21]. Among the several mechanisms of the extrinsic contribution, the one arising from the band-off-diagonal elements of the out-of-equilibrium single-carrier density matrix [32,33] has attracted much recent attention [27,34–36]. Resorting to the density-matrix transport theory in the weak disorder-potential regime [32,34,37] with a well-defined multiband structure [38], this mechanism contributes a spin current in the form [39]

$$\mathbf{j}^{s,\mathrm{ex}}=\sum_{l}g_{l}^{(-2)}\mathbf{j}_{l}^{s,\mathrm{ex}}. \tag{9}$$

Here, $g_{l}^{(-2)}$ is just the conventional out-of-equilibrium distribution function in the Boltzmann transport theory, in the order

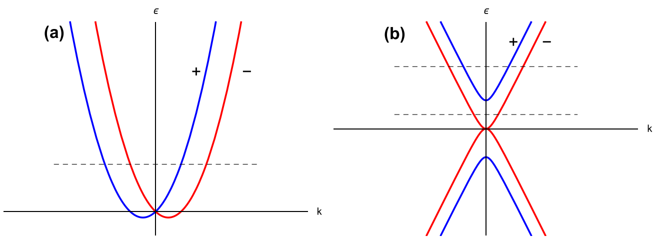

FIG. 1. Schematic of the band structures of the (a) 2D Rashba model and (b) 2D Dirac-Rashba model.

of $\langle V^2\rangle^{-1}$ with V the disorder potential. $l = (\eta, \mathbf{k})$ where η is the band index and $\mathbf{k}$ is the momentum. In the case of a scalar disorder potential $[\hat{\mathbf{r}}\hat{s}_z, \hat{V}(\hat{\mathbf{r}})] = 0$, we get [37]

$$\mathbf{j}_l^{s,\mathrm{ex}} = \sum_{l'} \omega_{l'l}^{(2)} \left(\mathbf{A}_{l'}^s - \mathbf{A}_l^s\right), \tag{10}$$

when $s_z^l \equiv \langle u_l|\hat{s}_z|u_l\rangle = 0$. The expression of $\mathbf{j}_l^{s,\mathrm{ex}}$ in the case of $s_z^l \neq 0$ is given in the Supplemental Material [37]. Here, $\mathbf{A}_l^s \equiv i\langle u_l|\hat{s}_z|\partial_{\mathbf{k}} u_l\rangle$, $|l\rangle \equiv |\mathbf{k}\rangle|u_l\rangle$ is the eigenstate of the disorder-free equilibrium Hamiltonian $\hat{H}_0^{\mathrm{eq}}$ with energy ϵ_l, and $\omega_{l'l}^{(2)} = \frac{2\pi}{\hbar}\langle|V_{ll'}|^2\rangle\delta(\epsilon_l - \epsilon_{l'})$ is the lowest-Born-order scattering rate. Since $s_z^l = 0$, $\mathbf{A}_l^s$ is real and remains unchanged under a local $U(1)$ gauge transformation $|u_l\rangle \to e^{i\phi_l}|u_l\rangle$. The extrinsic contribution Eq. (9) can be independent of both the disorder potential and impurity density, and thus may cancel partly or totally the intrinsic SHE.

In the weak disorder-potential regime, other disorder-induced contributions to the SHE [27,35,36,40] vanish in the presence of weak scalar scattering when the Berry curvatures on the Fermi surfaces are zero. This can be appreciated most easily in the limit of a smooth disorder potential varying slowly on the scale of the lattice constant [41]. Thus the disorder-induced SHE is just given by Eq. (9). This is the case in 2D systems with Rashba spin-orbit interactions, which are the focus of the following model analysis.

We first apply the above results to the 2D Rashba model [both Rashba subbands partially occupied, Fig. 1(a)] with smooth scalar-impurity potentials, arriving at vanishing SHE (see Supplemental Material [37]), consistent with previous works [20,21]. According to the generalized Mott relation, the SNE of the SZXN current vanishes.

Now we discuss a model showing nonzero SHE and SNE of the SZXN current. As a minimal model for low-energy electronic states around the Dirac point K in a graphene monolayer subject to a $z \to -z$ asymmetric spin-orbit interaction, the 2D Dirac-Rashba Hamiltonian in the A-B sublattice space reads [42]

$$\begin{aligned}\hat{H}_0^{\mathrm{eq}} =& v\begin{bmatrix} 0 & (k_x - ik_y)\sigma_0 \\ (k_x + ik_y)\sigma_0 & 0 \end{bmatrix} \\ &+ \lambda_R \begin{bmatrix} 0 & \sigma_y + i\sigma_x \\ \sigma_y - i\sigma_x & 0 \end{bmatrix}.\end{aligned} \tag{11}$$

Here, $v = \hbar v_F$, σ_i $(i = x, y, z)$ is the Pauli matrix and σ_0 the unit matrix in the spin space, and λ_R is the Rashba coupling. The four bands of $\hat{H}_0^{\mathrm{eq}}$ read $\epsilon_k^{\eta\zeta} = \eta[\sqrt{\lambda_R^2 + (vk)^2} + \zeta\lambda_R]$. Here, $\eta = \pm 1$ denote conduction or valence bands, and $\zeta = \pm 1$ denote spin subbands. We only consider the n-doped case [Fig. 1(b)].

TABLE I. The intrinsic ($\sigma_{yx}^{s,\mathrm{in}}$) and extrinsic ($\sigma_{yx}^{s,\mathrm{ex}}$) spin Hall conductivities in the case of both conduction bands partially occupied ($\epsilon_F > 2\lambda_R$) and of an empty inner conduction band ($\epsilon_F < 2\lambda_R$) in the 2D Dirac-Rashba model.

	$\epsilon_F > 2\lambda_R$	$\epsilon_F < 2\lambda_R$
$\sigma_{yx}^{s,\mathrm{in}}$	$-\frac{3e}{8\pi}\frac{\epsilon_F^2-2\lambda_R^2}{\epsilon_F^2-\lambda_R^2}$	$-\frac{e}{16\pi}\frac{2\epsilon_F^2+\lambda_R\epsilon_F+2\lambda_R^2}{\lambda_R(\epsilon_F+\lambda_R)}$
$\sigma_{yx}^{s,\mathrm{ex}}$	$-\frac{e}{8\pi}\frac{\epsilon_F^2-2\lambda_R^2}{\epsilon_F^2-\lambda_R^2}$	$-\frac{e}{16\pi}\frac{\epsilon_F+2\lambda_R}{\epsilon_F+\lambda_R}$
$\sigma_{yx}^s = \sigma_{yx}^{s,\mathrm{in}} + \sigma_{yx}^{s,\mathrm{ex}}$	$-\frac{e}{2\pi}\frac{\epsilon_F^2-2\lambda_R^2}{\epsilon_F^2-\lambda_R^2}$	$-\frac{e}{8\pi}\frac{\epsilon_F^2+\lambda_R\epsilon_F+2\lambda_R^2}{\lambda_R(\epsilon_F+\lambda_R)}$

For the intrinsic SHE, a lengthy but straightforward calculation leads to the results presented in Table I. In the presence of a smooth scalar disorder potential the intervalley scattering is suppressed, thus we obtain

$$\left(\mathbf{j}_l^{s,\mathrm{ex}}\right)_y = -\frac{\hbar}{4}\frac{\hbar v_F}{\epsilon_l}\sin\xi\,\frac{1}{\tau_l^{\mathrm{tr}}}\cos\phi \tag{12}$$

in Eq. (9), where we use $(\mathbf{A}_{\eta\zeta\mathbf{k}}^s)_y = \eta\frac{\hbar}{4}\frac{\hbar v_F}{\epsilon_l}\sin\xi\cos\phi$ ($s_z^l = 0$ in this model) with $\sin\xi = vk/\sqrt{\lambda_R^2 + (vk)^2}$ and $\tan\phi = k_y/k_x$. $\tau_l^{\mathrm{tr}} = 1/\sum_{l'}\omega_{l'l}^{(2)}[1 - \cos(\phi' - \phi)]$ is the transport time in the case of smooth scalar disorder. The out-of-equilibrium distribution function reads

$$g_l^{(-2)} = \frac{e}{\hbar}\mathbf{E}\cdot(-\partial f^0/\partial\mathbf{k})\tau_l^{\mathrm{tr}}, \tag{13}$$

thus Eq. (9) yields the extrinsic SHE listed in Table I. The total spin Hall conductivity σ_{yx}^s is positive definite and depends on the Fermi energy, as shown in Table I.

The spin Nernst conductivity $\alpha_{yx}^s = L_{yx}^{sQ}(T, \mu)/T$ is obtained by the Mott relations (7) and (8). In particular, in the case of strong Rashba spin-orbit interactions, the chemical potential may be located in the region $2\lambda_R \gg \mu \gg k_B T$ ($\epsilon_{k=0}^{++} = 2\lambda_R$) at low temperatures, then the standard Mott relation (8) applies, yielding

$$\frac{\alpha_{yx}^s}{T} = -\frac{\pi k_B^2}{24\lambda_R}\left[1 - \frac{3\lambda_R^2}{(\mu + \lambda_R)^2}\right]. \tag{14}$$

This spin Nernst conductivity displays a sign change at $\mu/\lambda_R = \sqrt{3} - 1$.

Discussion. The SZXN spin current has been proved to obey the basic near-equilibrium transport relations, i.e., the Mott relation established above and the Onsager relation shown previously [12,14]. On the other hand, for a conventional spin current defined as the anticommutator of the velocity and spin operators, whether or not the Mott relation is valid (when the transported spin is nonconserved) is still a problem not completely settled in the literature. Here, we discuss this issue, because a conventional spin current is frequently used in theoretical formulations of spin transport [1], although it is not directly related to the transport of spin in the case of spin nonconservation [43]. Accordingly, in this case it is expected that the Mott relation as a transport relation does not apply for a conventional spin current. We point out that existing theories indeed do not prove the Mott relation for conventional spin currents. Moreover, a recent work showed the breakdown of the Mott relation for a conventional spin current in a specific model [7].

The direct application of the Kubo-Luttinger-Streda formalism presented in this study to the thermoelectric response of a conventional spin current does not yield the generalized Mott relation when the transported spin component is not conserved. For the SNE of the conventional spin current, the conventional-spin-current–heat-current correlation function reads [37] ($D_{yx}^{s0e} \equiv \sigma_{yx}^{s0}$)

$$D_{yx}^{s0Q}(T,\mu) = \int d\epsilon\left[-\frac{df^0(\epsilon)}{d\epsilon}\right]\frac{(\epsilon-\mu)}{e}\sigma_{yx}^{s0}(T=0,\epsilon) - \frac{1}{e}\int d\epsilon f^0(\epsilon)\sigma_{yx}^{s0,II}(T=0,\epsilon). \tag{15}$$

However, $M_{yx}^{s0Q}(T,\mu)+D_{yx}^{s0Q}(T,\mu)$ cannot yield the Mott relation generally because $M_{yx}^{s0Q}(T,\mu)$ cannot be expressed as a Fermi sea integral of the so-called "Fermi sea term" [1,44] $\sigma_{yx}^{s0,II}(T=0,\epsilon)$ of conventional spin Hall conductivity. If one calculated only the spin-current–heat-current correlation function D_{yx}^{s0Q} and neglected concurrently the Fermi sea term $\sigma_{yx}^{s0,II}$ of the spin Hall conductivity, it would be concluded that the Mott relation is valid for a conventional spin current. But this is not correct because generally both of these two contributions are important [22,45].

In the 2D Rashba model with scalar disorder, $\sigma_{yx}^{s0}=0$ [46] and thus

$$D_{yx}^{s0Q} = -\frac{1}{e}\int d\epsilon f^0(\epsilon)\sigma_{yx}^{s0,II}(T=0,\epsilon). \tag{16}$$

The disorder-free part (that dominates $\sigma_{yx}^{s0,II}$ in the weak disorder-potential regime [1]) of $\sigma_{yx}^{s0,II}$ is calculated to be $\sigma_{yx}^{s0,II}(T=0,\epsilon)=\frac{e}{8\pi}(\frac{k_R}{k_0(\epsilon)}-\frac{k_0(\epsilon)}{k_R})\theta(-\epsilon)$, with θ the step function and $k_0(\epsilon)=\alpha_R^{-1}\sqrt{\epsilon_R^2+2\epsilon_R\epsilon}$. Therefore, in the low-temperature limit $D_{yx}^{s0Q}(T\to 0)=-\frac{\epsilon_R}{12\pi T}$ is divergent when both Rashba subbands are partially occupied. Recently, Dyrdal *et al.* [7] directly evaluated the bubble [3] and vertex corrections of $D_{yx}^{s0Q}(T,\mu)$ in the Rashba model, and obtained the same low-temperature-limit value. They introduced a spin-resolved orbital magnetization by hand and argued that this quantity also contributes a spin current that should be added to the result of the conventional-spin-current–heat-current correlation function [7]. This treatment removes the divergent value of D_{yx}^{s0Q} in the zero-temperature limit in the Rashba model [7], but yields a SNE which does not follow the generalized Mott relation for conventional spin currents.

In summary, we proved the Mott relation for the spin thermoelectric transport with the SZXN definition of the spin current. First-principles calculations of the intrinsic SHE in terms of the SZXN current have been available in specific materials such as some nonmagnetic hcp metals where the spin-nonconserving part of the spin-orbit interaction could be important [17]. Thus a first-principles prediction of the intrinsic SNE according to the Mott relation in these materials can be made.

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